Coupling Grain Scale and Bulk Mechanical Response of PBXs via Numerical Simulation

Scott Bardenhagen and Andrew Brydon, T-14

The mechanical response of Plastic-Bonded Explosives (PBXs) is of interest in a variety of munitions and industrial applications. PBXs are composed of energetic grains embedded in a polymeric binder. The heterogeneity at this material scale localizes energy during deformation, resulting in damage nucleation sites and hot spots. Continuum models have been developed to estimate bulk material response, but because there is little connection to the grain scale physics, these models cannot be applied far from their calibrated regime with confidence. To develop predictive models, it is imperative to develop a sound physical understanding of grain scale material response and incorporate the appropriate physics in PBX continuum constitutive models. The Stochastic Transformation Field Analysis (STFA) is a continuum constitutive model that incorporates detailed grain scale information. The STFA develops governing equations applicable to a variety of heterogeneous materials, but requires (grain scale) strain heterogeneity statistics for calibration. This calibration is supplied using numerical simulations of PBXs.

Numerical simulation has been used to extract bulk material properties in a manner analogous to traditional "physical" experiments. In order for the simulations to give repeatable results, they must include a sufficient quantity of material, denoted a "Representative Volume Element" (RVE). For bulk properties, such as moduli, it has been found that good estimates may be obtained with surprisingly small RVEs. Here numerical simulations are used to determine the RVE size for both bulk properties and strain state statistics. The study is performed for detailed geometries and material properties appropriate to PBX-9501, a specific composition of interest at the Laboratory.

A particle method is chosen for performing simulations because of its compatibility with discretization of complex geometries determined experimentally. Samples are extracted from an x-ray microtomography data set and subjected to uniaxial compression. Figure 1 depicts representative grain configurations for the three sample sizes considered; a binder fills the interstitial regions. Bulk composite elastic properties are determined by measuring confining forces during compression. It was found that moduli were accurately estimated (within 1%) using the smallest sample size.

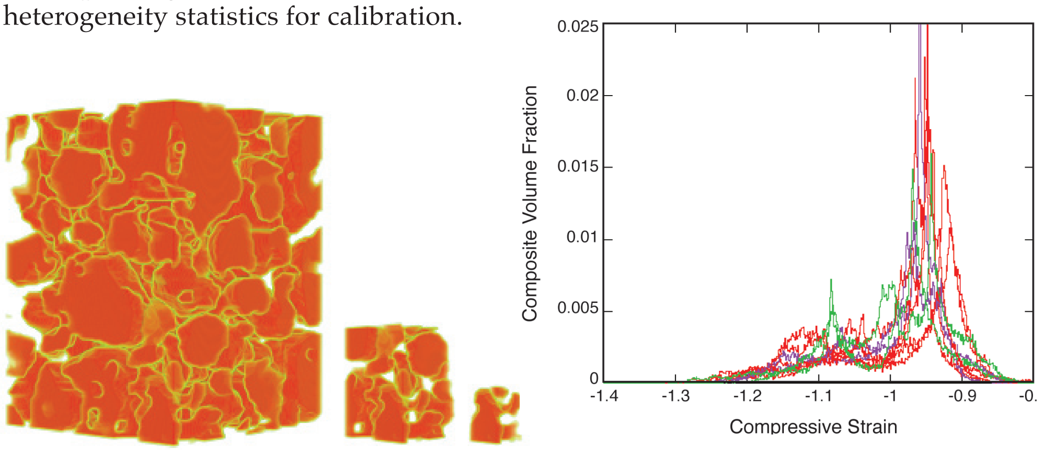
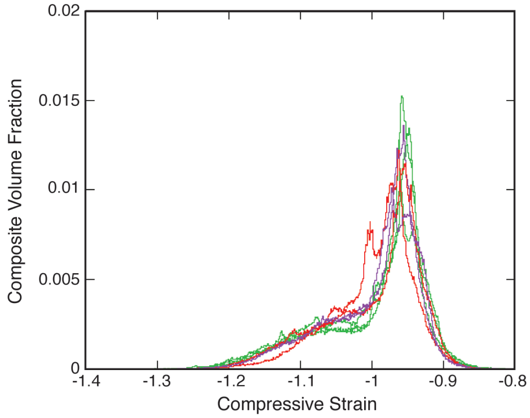


Fig. 1. *Three material sample sizes used in RVE study (left) and small sample size compressive strain state distributions (nine realizations).*



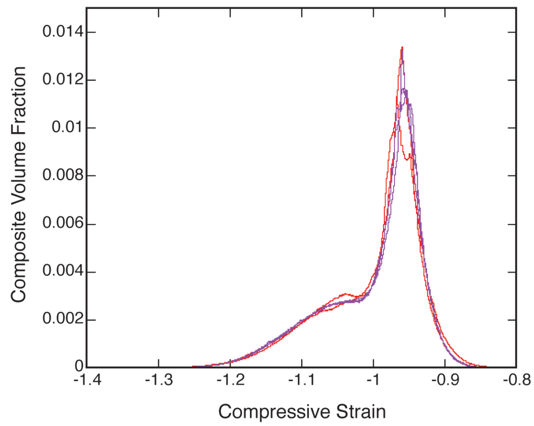


Fig. 2.
Compressive strain state distributions for the medium (left) and large sample sizes (seven and five realizations, respectively).

Figure 1 also depicts histograms of the normalized compressive strain for computations on nine small sample size realizations of grain scale structure. Substantial variation in strain distribution is evident. Results for the medium sample size are depicted in Fig. 2. The general similarity of most of the histograms suggests convergence. However, outliers remain, and the definition of the peak is unsatisfactory. Results for the large sample size are also depicted in Fig. 2. While some variation between samples near the peak remains, the general convergence of the histograms suggests that the large sample sizes are statistically representative of PBX-9501. The strain state statistic RVE has physical dimensions 0.39 x 0.39 x 0.53 mm^3, and is approximately one hundred times larger than a bulk property RVE.

The combination of detailed grain scale morphology determined using x-ray microtomography, statistics generated by computations, and a constitutive modeling approach calibrated using these statistics, provides a methodology to include more detailed information in continuum constitutive models of PBX-9501.

For more information contact
Scott Bardenhagen at bard@lanl.gov.